Chapter Three
Matrix Formulation of Quantum Mechanics

A special abbreviated notations has used by Paul Dirac to rephrasing rules and so ideas of quantum mechanics. These notations, together with the sense of Hilbert space, have been provide a successful complete abstract formulation for the quantum mechanics. Hence, another simple analog manipulation could replace the common analytical one. In fact, this approach may compensated and spare the difficulty usually associated with the conventional procedure.

3-1 Abstract View of Quantum Mechanics

According to the thoughts mentioned above the complete orthonormal eigen wave functions for any quantum mechanical system are regarded to serve as a BAISES vectors in Hilbert space (linear vector space). In Dirac notation, each of these functions, say u_n, is represented by a KET state vector $|n\rangle$. So, the completeness principle in this notation becomes;

$$|\varphi\rangle = \sum_n c_n |n\rangle \qquad \ldots (3\text{–}1)$$

Where $|\varphi\rangle$ is a common state vector, c_n is the project of $|\varphi\rangle$ on the ket vector $|n\rangle$. Now, if a given set of ket vectors $|1\rangle, |2\rangle, \ldots, |n\rangle$ can be used to represent any vector $|\varphi\rangle$ that belongs to the vector space H (quantum mechanical system). It is obvious that the set $\{|n\rangle\}$ *spans* the given vector space.

H.W: *Find the matrix for of each ket vector $|n\rangle$ in equation (3-1), in other word show that the ket vectors $|n\rangle$ spans Hilbert's space. i.e. synthesis all of the allowed states of QM system.*

From equation (3-1) we may get;

$$c_n = \langle n|\varphi\rangle \qquad \ldots (3\text{–}2)$$

The substitution of the project c_n in the completeness principle leads to;

$$|\varphi\rangle = \sum_n |n\rangle\langle n|\varphi\rangle \qquad \ldots (3\text{–}3)$$

Since the last equation must be valid for any ket vector $|\varphi\rangle$ it follows that;

$$\sum_n |n\rangle\langle n| = \hat{1} \qquad \ldots (3\text{–}4)$$

Where $\hat{1}$ is a unit operator usually called ***identity operator***. It has the property that when it acts on a state vector leave it without change. Equation (3-4) also called ***completeness relation*** or ***closure relation***.

H.W: *Show that the ket vectors forms a complete orthonormalized set.*

Notes:

i- Actually there will be a space of conjugate associated with the space of kets described by bras and related to each other by;

$$\langle\varphi| = |\varphi\rangle^* \qquad \ldots (3\text{–}5)$$

Thus from equation (3-1) one may get;

$$\langle\varphi| = \sum_n c_n^* \langle n| \qquad \ldots (3\text{–}6)$$

ii- The overlap integral (inner product) of the two state vectors $|\varphi\rangle$ and $|\psi\rangle$ may formulate as follows;

$$\langle\varphi|\psi\rangle = \sum_m \sum_n c_m^* \, b_n \langle m|n\rangle$$

$$\langle\varphi|\psi\rangle = \sum_m \sum_n c_m^* \, b_n \delta_{mn}$$

$$\langle\varphi|\psi\rangle = \sum_n c_n^* \, b_n \qquad \ldots (3\text{–}7)$$

Obviously, it follows that;

$$\langle\varphi|\psi\rangle^* = \langle\psi|\varphi\rangle \qquad \ldots (3\text{–}8)$$

iii- The outer product of the two state vectors $|\varphi\rangle$ and $\langle\psi|$, namely $|\varphi\rangle\langle\psi|$, is an operator which when acts on the state vector like $|\chi\rangle$ leads to a new state vector. i.e. $(|\varphi\rangle\langle\psi)|\chi\rangle = \alpha|\varphi\rangle$ where α is a complex number.

iv- For any operator $\hat{A}$ there being an associated operator denoted by $\hat{A}^\dagger$, called Hermitian conjugate (adjoint) operator, and defined as follows;

$$\langle\varphi|\hat{A}^\dagger|\psi\rangle = \langle\psi|\hat{A}|\varphi\rangle^* \qquad \ldots (3\text{–}9)$$

Or equivalently;

$$\langle\varphi|\hat{A}^{\dagger}|\psi\rangle^{*} = \langle\psi|\hat{A}|\varphi\rangle$$

At a time when $\hat{A}$ acts upon ket vectors from the left, $\hat{A}^{\dagger}$ acts upon bra vectors from the right, and they lead to transform them into a new ket and bra vectors respectively. For instance, if;

$$\hat{A}|\phi\rangle = |\hat{A}\phi\rangle = |\psi\rangle \qquad \ldots \text{ (3–10a)}$$

We find;

$$(\hat{A}|\phi\rangle)^{*} = \langle\varphi|\hat{A}^{\dagger} = \langle\hat{A}\varphi| = \langle\psi| \qquad \ldots \text{ (3–10b)}$$

v- For the case when $\hat{A} = \hat{A}^{\dagger}$, the operator $\hat{A}$ is called Hermitian (self adjoint). So, in sense of equation (3-9) we get the following Hermitian relation;

$$\langle\varphi|\hat{A}|\psi\rangle = \langle\psi|\hat{A}|\varphi\rangle^{*} \qquad \ldots \text{ (3–11)}$$

H.W:

1- Show that by taking the Hermitian conjugate twice one may get back to the same operator. i.e. $(\hat{A}^{\dagger})^{\dagger} = \hat{A}$.

2- Prove that for Hermitian operator $\hat{A}^{\dagger} = \hat{A}$.

3- Use the definition ($\langle\psi|\hat{A}\psi\rangle = \langle\hat{A}^{\dagger}\psi|\psi\rangle$) for the Hermitian conjugate (adjoint) operator to derive the general formula for the Hermitian operator (self-adjoint) ($\langle\chi|\hat{A}\varphi\rangle = \langle\hat{A}\chi|\varphi\rangle$). **Hint**; assume that $|\psi\rangle = |\phi\rangle + \lambda|\chi\rangle$.

4- Prove that: $(\lambda\hat{A})^{\dagger} = \lambda^{*}\hat{A}^{\dagger}$.

5- Prove that: $(\hat{A}\hat{B})^{\dagger} = \hat{B}^{\dagger}\hat{A}^{\dagger}$.

6- Prove that: $(\hat{A} + \hat{B})^{\dagger} = \hat{A}^{\dagger} + \hat{B}^{\dagger}$

7- Evaluate the outer product $|1\rangle\langle 1|$ and $|1\rangle\langle 2|$.

8- Find the adjoint of the operator $\hat{A} = \alpha|1\rangle\langle 0| - \beta|0\rangle\langle 1|$

3 -2 Projection Operator

The operator $|n\rangle\langle n|$ is called projection operator and it is defined by;

$$P_n = |n\rangle\langle n| \quad \ldots (3\text{–}12)$$

Which has the property;

$$P_m P_n = |m\rangle\langle m|n\rangle\langle n|$$

$$P_m P_n = \delta_{mn}|m\rangle\langle n|$$

$$P_n P_n = P_n \quad \ldots (3\text{–}13)$$

Keeping in mind;

$$\sum_n P_n = \hat{1}$$

Actually, equation (3-13) announce that;

$$P_n^2 = P_n$$

The name projection operator is come from the property that when such an operator acting on arbitrary ket $|\psi\rangle$, it will projects it into the eigen ket $|n\rangle$ with a probable amplitude $\langle n|\psi\rangle$, or partial probability density equal to $|\langle n|\psi\rangle|^2$. Another results could be read from equation (3-13), that is once a common state vector $|\psi\rangle$ is projected into a particular base (eigen ket) $|n\rangle$, then no more changes could be happened if a further projection be done.

Actually, such a property for P_n is completely matches with the distribution of what a measurement process being. For example let's assume we wont to measure the energy of a quantum mechanical system which described by the state vector $|\psi\rangle$ {also one may say a collection of systems all of which are described by the same vector $|\psi\rangle$}. The measuring process we doing means that we are picking a one eigen ket {a one of these collection}, like $|n\rangle$, and measuring its energy. Along with finding a particular result, E_n with a probability $|\langle n|\psi\rangle|^2$, the measurement must change the vector $|\psi\rangle$ so that it end up to the eigen ket vector $|n\rangle$. The reason behind is that subsequent measurements in that vector $|\psi\rangle$ can only give the same result over and over again. Thereby, the energy expectation value become;

$$\langle\psi|\hat{H}|\psi\rangle = \sum_n |\langle n|\psi\rangle|^2 \, E_n$$

$$\langle\psi|\hat{H}|\psi\rangle = \sum_n \langle\psi|n\rangle \, E_n \langle n|\psi\rangle \qquad \ldots \text{(3–14)}$$

Equation (3-14) state that, operator $\hat{H}$ could be written in terms of its eigen values and their corresponding projects as follows;

$$\hat{H} = \sum_n P_n \, E_n \qquad \ldots \text{(3–15)}$$

H.W:

1- Prove that the projector operator is Hermitian (self adjoint).

2- Determine the conditions by means the product of any two projector operators is also a projector operator.

3- Check whether the operator $|n\rangle\langle n| - i|n\rangle\langle m| + i|m\rangle\langle n| - |m\rangle\langle m|$ is projector or not.

3-3 Matrix Representation of Operator

In the previous course we learned a simple approach to formulate operators, and so wave functions, in terms of matrices depending on the analogy with mathematical vectors. Now we would explore another advanced one to do so in accordance with the ideas mentioned in the previous section. Anyway, let's start, as example, with following relation;

$$\hat{a}^{+}|n\rangle = \sqrt{n+1}|n+1\rangle \qquad \ldots \text{(3–16)}$$

Where $|n\rangle$ is any of the complete orthonormal eigen ket vectors for the quantum harmonic oscillator system. Now, by take the scalar product for this equation with $\langle m|$ we can get;

$$\langle m|\hat{a}^{+}|n\rangle = \sqrt{n+1}\delta_{m,n+1} \qquad \ldots \text{(3–17)}$$

Obviously the regards of all admissible values of n and m leads to arrange equation (3-17) in the form of array or matrix. The conventional notation of a matrix M_{ij} has the first index labeling the row and the second labeling the column of the array. Accordingly if we write $\langle m|\hat{a}^{+}|n\rangle$ as $\hat{a}^{+}{}_{mn}$ we find;

$$\hat{a}^{+}{}_{mn} = \begin{pmatrix} 0 & 0 & 0 \ldots \\ \sqrt{1} & 0 & 0 \cdots \\ 0 & \sqrt{2} & 0 \cdots \\ 0 & 0 & \sqrt{3} \ldots \\ \vdots & \vdots & \vdots \end{pmatrix} \qquad \ldots (3\text{–}18)$$

So without loss for the specialty we can call $\langle m|\hat{A}|n\rangle$, where $\hat{A}$ is any operator and $|n\rangle$ any complete set of states, a matrix representation of $\hat{A}$ in terms of the basis provided by the complete set of states $|n\rangle$.

The above appellation needs some justification, so we try the following;

1) Conventionally the multiplication of two matrices is define as follows;

$$(AB)_{ij} = \sum_n (A)_{in}\,(B)_{nj} \equiv (A)_{in}(B)_{nj} \qquad \ldots (3\text{–}19)$$

So, it is necessary to verify that this relation holds good for the matrix representation of the operators $\hat{A}$ and $\hat{B}$. To do so let's expand the state $\hat{B}|j\rangle$ in terms of the complete eigen kets $|n\rangle$ as follows;

$$\hat{B}|j\rangle = \sum_n c_n\,|n\rangle \qquad \ldots (3\text{–}20)$$

Where $c_n = \langle n|\hat{B}|j\rangle$. So equation (3-20) became;

$$\hat{B}|j\rangle = \sum_n |n\rangle\,\langle n|\hat{B}|j\rangle \qquad \ldots (3\text{–}21)$$

Hence;

$$\langle i|\hat{A}\hat{B}|j\rangle = \sum_n \langle i|\hat{A}|n\rangle\,\langle n|\hat{B}|j\rangle \qquad \ldots (3\text{–}22)$$

It is seen that equation (3-22) is the same as equation (3-19) provided that $\langle i|\hat{A}|n\rangle = (\hat{A})_{in}$ and $\langle n|\hat{B}|j\rangle = (\hat{B})_{nj}$.

2) Further justification for matrix representation come from the definition of hermitian conjugate operator given by;

$$\langle m|\hat{A}|n\rangle^{*} = \langle \hat{A}m|n\rangle = \langle n|\hat{A}^{\dagger}|m\rangle \qquad \ldots (3\text{–}23)$$

Which shows that if the operator $\hat{A}$ is represented by a matrix, then the hermitian conjugate operator $\hat{A}^{\dagger}$ will be represented by the herrmitian conjugate matrix, since the latter is defined by

$$(\hat{A}^{\dagger})_{nm} = (\hat{A}^{*})_{mn} \qquad \ldots (3\text{–}24)$$

3-4 Space Transformation of Operators

Suppose that the complete set of kets $|v_n\rangle$, are an eigen kets of an operators like $\hat{A}$, then the matrix representation of this operator is;

$$\langle v_m|\hat{A}|v_n\rangle = a_n\delta_{mn} = a_m\delta_{mn} \qquad \ldots (3\text{–}25)$$

An example for such operators is the Hamiltonian of harmonic oscillator that satisfy the following eigen value equation;

$$\widehat{H}|n\rangle = \hbar\omega\left(n+\frac{1}{2}\right)|n\rangle \qquad \ldots (3\text{–}26)$$

However, adoption of equation (3-25) leads to write equation (3-26) in the following matrix form;

$$\langle m|\widehat{H}|n\rangle = \hbar\omega\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0\cdots \\ 0 & \frac{3}{2} & 0 & 0\cdots \\ 0 & 0 & \frac{5}{2} & 0\cdots \\ 0 & 0 & 0 & \frac{7}{2}\cdots \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix} \qquad \ldots (3\text{–}27)$$

It is quite obvious that the determination of the eigen values of a hermitian operator is equivalent to diagonalizing its correspondent matrix. In other word, the problem of finding the eigen values for an operator expressed in terms of its complete set of orthonormal eigenkets is tantamount to digonalizing its correspondence matrix. The question now is how we could make the digonalizaition process when such an operator is given in terms of a set of orthonormal kets but this set is not eigen kets for this operator.

Let us consider the operator $\hat{A}$ whose eigen kets are $|v_n\rangle$. Further, suppose we know the matrix elements of $\hat{A}$ in a basis $|u_n\rangle$, that is we know each entry in the square matrix;

$$A_{mn} = \langle u_m|\hat{A}|u_n\rangle \qquad \ldots (3\text{–}28)$$

According to the completeness principle, an arbitrary eigen kets $|v_n\rangle$ may be expand in terms of the basis $|u_n\rangle$. So,

$$|v_n\rangle = \sum_k |u_k\rangle\langle u_k|v_n\rangle \qquad \ldots (3\text{–}29)$$

And so,

$$\langle v_n| = \sum_l \langle v_n|u_l\rangle \langle u_l| \qquad \ldots (3\text{–}30)$$

Therefore, equation (3-25) becomes;

$$a_m\delta_{mn} = \langle v_m|\hat{A}|v_n\rangle$$

$$a_m\delta_{mn} = \sum_l \quad \sum_k \langle v_m|u_l\rangle\langle u_l|A|u_k\rangle\langle u_k|v_n\rangle$$

$$a_m\delta_{mn} = \sum_{l,k} \langle v_m|u_l\rangle\langle u_l|A|u_k\rangle\langle u_k|v_n\rangle \qquad \ldots (3\text{–}31)$$

If we define that; $U_{kn} = \langle u_k|v_n\rangle$, where;

$$\langle u_l|v_m\rangle^* = \langle v_m|u_l\rangle$$

$$U_{lm}{}^* = U_{ml}{}^\dagger \qquad \ldots (3\text{–}32)$$

Then equation (3-31) can be written as;

$$a_m\delta_{mn} = \sum_{l,k} U_{ml}{}^\dagger A_{lk} U_{kn}$$

$$a_m\delta_{mn} = \sum_l \quad \sum_k U_{ml}{}^\dagger A_{lk}\, U_{kn}$$

$$a_m\delta_{mn} = (U^\dagger A U)_{mn} = A_{mn} \qquad \ldots (3\text{–}33)$$

Absolutely equation (3-33) emphases the fact that we are make a transformation for the matrix elements of operator $\hat{A}$ from the space $|u_n\rangle$ to the space $|v_n\rangle$. For this reason matrix U_{kn} is called transformation matrix. However, due to the property of U_{kn} that is;

$$U^\dagger U = 1 \qquad \ldots (3\text{–}34)$$

This matrix is called unitary transformation matrix and we can easily prove that.

It should be mentioned that when the matrix $\langle v_m|A|v_n\rangle$ is hermitian, then that matrix $\langle u_m|A|u_n\rangle$ will be hermitian too. In other word, the hermitian property for a matrix being conserved without change after transformation process.

H.W:

1) Prove that $U^\dagger U = 1$.

2) Prove the conservation of the transformation property.

It is often useful to define the summation of diagonal elements of a matrix to be the trace of that matrix. i.e.

$$TrA = \sum_n A_{nn} \qquad \ldots (3\text{–}35)$$

Accordingly one may say the trace of operator $\hat{A}$ is;

$$TrA = \sum_n \langle n|A|n\rangle \qquad \ldots (3\text{–}36)$$

Which tends directly to the form given by equation (3-35). Anyway, the trace of a product of two matrices has a useful characteristic that is;

$$TrAB = TrBA \qquad \ldots (3\text{–}37a)$$

Which can be proved easily as follows;   enhance review

$$TrAB = \sum_n (AB)_{nn}$$

$$TrAB = \sum_n \sum_m A_{nm}\, B_{mn}$$

Since A_{nm} and B_{mn} are just a numbers, so we could change the order regarding the commutation property of multiplication and so;

$$TrAB = \sum_m \sum_n B_{mn} A_{nm}$$

$$TrAB = \sum_m (BA)_{mm} = TrBA$$

From another point of view we can justifying the identity (3-37a) by another approach considering the operator in equation (3-11) as follows;

$$TrAB = \sum_n \langle n|AB|n\rangle = \sum_n \langle n|A\hat{1}B|n\rangle$$

$$TrAB = \sum_n \quad \sum_m \langle n|A|m\rangle\langle m|B|n\rangle$$

$$TrAB = \sum_m \quad \sum_n \langle m|B|n\rangle\langle n|A|m\rangle$$

$$TrAB = \sum_m \langle m|B\hat{1}A|m\rangle$$

$$TrAB = \sum_m \langle m|BA|m\rangle$$

$$TrAB = TrBA$$

H.W: Prove that *TrABC=TrBCA* .... (3–37b)

Equation (3-37a) implies an important fact that;

$$Tr[A,B] = 0 \qquad \ldots (3\text{–}38)$$

Keeping in mind the polynomial in equation (3-35) must be convergence. Otherwise equation (3-38) being not valid and so no useful consequence can be mention. ***Thereby, for finite dimensional matrices their own traces must finite, while for infinite dimension matrices are not***. An examples for the first kind are the matrices of angular momentum, that are deduced from the definition $\hat{L} = \hat{r} \times \hat{p}$, namely;

$$[\hat{\ell}_x, \hat{\ell}_y] = i\hbar\hat{\ell}_z \quad .....(a)$$

$$[\hat{\ell}_y, \hat{\ell}_z] = i\hbar\hat{\ell}_x \quad .....(b) \qquad \text{(Prove)} \qquad ...\ (3\text{–}39)$$

$$[\hat{\ell}_z, \hat{\ell}_x] = i\hbar\hat{\ell}_y \quad .....(c)$$

Their counterpart, however, for the second type are;

$$[\hat{p}_x, \hat{x}] = -i\hbar$$

$$[\hat{a}, \hat{a}^+] = 1 \qquad \text{(Prove)} \qquad ...\ (3\text{–}40)$$

Remark: All of the Hermitian operators have finite dimensional matrices while non-Hermitian operators are not.

3-5 Matrix Representation of Angular Momentum

3-5-1 Review for Some Basics

Before going in details for represent the angular momentum operators in matrices form, it is better to review some important facts that are covered previously in the M.Sc. course. Anyway, one really do know that incompatible observables are belong to operators which are not commute, so they obey to Heisenberg uncertainty principle. Evidently, incompatible observables do not have shared a same eigenvectors, or at least, they cannot have a complete set of common eigenvectors.

The Matrices that represents incompatible observables cannot simultaneously be diagonolized, that is, they cannot all be brought to diagonal form by the same similarity transformation. On the other hand, compatible observables, whose operators do commute, share a complete set of eigenvectors and hence their corresponding matrices can be simultaneously diagonolized.

The question now is whether the operators $\hat{H}$, $\hat{L}^2$, $\hat{\ell}_x$, $\hat{\ell}_y$ and $\hat{\ell}_z$ share a common complete set of eigenvectors or not. According to the last paragraph, this is possible if and only if these operators are commute with each other's. So, one has to review the following;

i) It had seen that the angular momentum is conserved observable for a systems have a central potentials. In other word it is a constant of motion. i.e. $d\hat{L}/dt = 0$, or equivalently;

$$[\hat{H}, \hat{L}] = 0 \qquad \text{. . . (3–40a)}$$

Or more precisely;

$$[\hat{H}, \hat{\ell}_x] = [\hat{H}, \hat{\ell}_y] = [\hat{H}, \hat{\ell}_z] = 0 \qquad \text{. . . (3–40b)}$$

ii) Obviously the components of angular momentum are commute with $\hat{L}^2$. i.e.

$$[\hat{\ell}_x, \hat{L}^2] = [\hat{\ell}_y, \hat{L}^2] = [\hat{\ell}_z, \hat{L}^2] = 0 \qquad \text{. . . (3–41)}$$

iii) The components of angular momentum are not commute with each other as indicated by equations (3-39).

It seen that, as a consequence for these remarks, only one component of $\hat{L}$ can be chosen together with $\hat{H}$ and $\hat{L}^2$ so as to form a simultaneously commuting set. Next question, however, is what will the component that may met such a goal. An objective answer for this question is that nothing may prevent from picking any one of them as a part of the commuting set. For conventional purposes the component $\hat{\ell}_z$ is usually picked keeping in mind there is nothing be special about this choice and hence any of the remaining ones could be choose instead. However, if the aspired eigenvectors are denoted by $|\ell m\rangle$ one may forward put the following eigen value equations;

$$\hat{L}^2|\ell m\rangle = \hbar^2 \ell(\ell + 1)|\ell m\rangle \qquad \text{. . . (3–42a)}$$

$$\hat{\ell}_z|\ell m\rangle = m\hbar|\ell m\rangle \qquad \text{. . . (3–42b)}$$

Where ℓ and m are just a real numbers since $\hat{L}^2$and $\hat{\ell}_z$ are hermitian operators and the presence of $\hbar$ is due to equations (3-39).

H.W: Prove that only the case for which $\hat{L} = 0$ could leads to have simultaneous eigenfunctions for all three components of the angular momentum. ***Hint: Assume that the set of functions*** $|u_n\rangle$ ***are forms a complete set for the three components and making use equation (3-39a).***

Solution:

Assume that the functions $|u_n\rangle$ forms a complete simultaneous commuting set, so:

$$\hat{\ell}_x|u_n\rangle = \ell_x^n|u_n\rangle$$

And,

$$\hat{\ell}_y|u_n\rangle = \ell_y^n|u_n\rangle$$

Thus it follow that;

$$\hat{\ell}_x\hat{\ell}_y|u_n\rangle = \ell_y^n\hat{\ell}_x|u_n\rangle$$

$$= \ell_y^n\ell_x^n|u_n\rangle$$

$$= \hat{\ell}_y\hat{\ell}_x|u_n\rangle$$

The substitution of the last equation in equation (3-39a) leads to the result;

$$\hat{\ell}_z|u_n\rangle = 0$$

So,

$$\ell_y^n|u_n\rangle = \hat{\ell}_y|u_n\rangle$$

$$= \frac{1}{i\hbar}[\hat{\ell}_z, \hat{\ell}_x]|u_n\rangle$$

$$= \frac{1}{i\hbar}(\hat{\ell}_z\hat{\ell}_x|u_n\rangle - \hat{\ell}_x\hat{\ell}_z|u_n\rangle)$$

$$= \frac{1}{i\hbar}(\ell_x^n\hat{\ell}_z|u_n\rangle - \hat{\ell}_x(0))$$

$$= \frac{1}{i\hbar}(\ell_x^n(0))$$

$$= 0$$

Similarly one may shows that $\ell_x^n|u_n\rangle = 0$ also, and thus it means that for $\hat{L} = 0$ could only have simultaneously eigenfunctions for all three components of the angular momentum.

3-5-2 Creative and Destructive Operator

The problem of what eigenvectors that forms a complete simultaneous computing set for the angular momentum operators ($\hat{\ell}_x$,$\hat{\ell}_y$, $\hat{\ell}_z$), $\hat{H}$ and $\hat{L}^2$, have been solved by chosen $\hat{\ell}_z$ as a part of commuting set. Where the desired eigenvector is named to be $|\ell m\rangle$ as indicated in equation (3-42). Next problem, however, is to explore what will happen when the residual components ($\hat{\ell}_x$,$\hat{\ell}_y$) coming to act upon $|\ell m\rangle$, which is the task of this context.

It customary to define the following two operators;

$$\hat{\ell}_+ = \hat{\ell}_x + i\hat{\ell}_y \qquad \ldots (3\text{–}43a)$$

$$\hat{\ell}_- = \hat{\ell}_x - i\hat{\ell}_y \qquad \ldots (3\text{–}43b)$$

Where they obey the following commutation relations;

$$[\hat{\ell}_+, \hat{\ell}_-] = [\hat{\ell}_x + i\hat{\ell}_y, \hat{\ell}_x - i\hat{\ell}_y]$$

$$[\hat{\ell}_+, \hat{\ell}_-] = -2i[\hat{\ell}_x, \hat{\ell}_y] = 2\hbar\hat{\ell}_z \qquad \ldots (3\text{–}44)$$

And so;

$$[\hat{\ell}_z, \hat{\ell}_\mp] = \hat{\ell}_z(\hat{\ell}_x \mp i\hat{\ell}_y) - (\hat{\ell}_x \mp i\hat{\ell}_y)\hat{\ell}_z$$

$$[\hat{\ell}_z, \hat{\ell}_+] = [\hat{\ell}_z, \hat{\ell}_x] \mp i[\hat{\ell}_z, \hat{\ell}_y]$$

$$[\hat{\ell}_z, \hat{\ell}_\pm] = i\hbar\hat{\ell}_y + i(\pm i\hbar)\hat{\ell}_x$$

$$[\hat{\ell}_z, \hat{\ell}_\mp] = \mp\hbar\hat{\ell}_\mp \qquad \ldots (3\text{–}45)$$

Furthermore it easy to prove that;

$$[\hat{L}^2, \hat{\ell}_\mp] = 0 \qquad \ldots (3\text{–}46)$$

Additionally one may write;

$$\hat{\ell}_+\hat{\ell}_- = (\hat{\ell}_x + i\hat{\ell}_y)(\hat{\ell}_x - i\hat{\ell}_y)$$

$$\hat{\ell}_+\hat{\ell}_- = \hat{\ell}_x{}^2 + \hat{\ell}_y{}^2 - i[\hat{\ell}_x, \hat{\ell}_y]$$

$$\hat{\ell}_+\hat{\ell}_- = \hat{L}^2 - \hat{\ell}_z{}^2 + \hbar\hat{\ell}_z \qquad \ldots (3\text{–}47a)$$

And similarly;

$$\hat{\ell}_-\hat{\ell}_+ = \hat{L}^2 - \hat{\ell}_z{}^2 - \hbar\hat{\ell}_z \qquad \text{(Prove)} \qquad \ldots (3\text{–}47b)$$

It , therefore, follows that;

$$\hat{L}^2 = \hat{\ell}_+\hat{\ell}_- + \hat{\ell}_z{}^2 - \hbar\hat{\ell}_z = \hat{\ell}_-\hat{\ell}_+ + \hat{\ell}_z{}^2 + \hbar\hat{\ell}_z \qquad \ldots (3\text{–}48)$$

In accordance with equations (3-42a) and (3-46) one may write;

$$\hat{L}^2\hat{\ell}_\pm|\ell m\rangle = \hat{\ell}_\pm\hat{L}^2|\ell m\rangle = \hbar^2\ell(\ell+1)\hat{\ell}_\pm|\ell m\rangle \qquad \ldots (3\text{–}49)$$

Obviously, equation (3-49) sate that the vector states $\hat{\ell}_\pm|\ell m\rangle$ are an eigen states for $\hat{L}^2$ with eigen value $\hbar^2\ell(\ell+1)$. On the other hand the consideration of equation (3-45) reads that;

$$\hat{\ell}_z\hat{\ell}_+|\ell m\rangle = (\hat{\ell}_+\hat{\ell}_z + \hbar\hat{\ell}_+)|\ell m\rangle$$

$$\hat{\ell}_z\hat{\ell}_+|\ell m\rangle = \hbar(m+1)\hat{\ell}_+|\ell m\rangle \qquad \ldots (3\text{–}50a)$$

Also one can get;

$$\hat{\ell}_z\hat{\ell}_-|\ell m\rangle = \hbar(m-1)\hat{\ell}_-|\ell m\rangle \qquad \ldots (3\text{–}50b)$$

It is clear that $\hat{\ell}_+|\ell m\rangle$ and $\hat{\ell}_-|\ell m\rangle$ are eigen state vectors for the operator $\hat{\ell}_z$ with an eigen value raised and lowered by unity respectively. For this reason, in fact, the operators $\hat{\ell}_+$ and $\hat{\ell}_-$ are called creative and destructive operators alternatively. Therefore, one may write;

$$\hat{\ell}_+|\ell m\rangle = C_+|\ell, m+1\rangle \qquad \ldots (3\text{–}51a)$$

$$\hat{\ell}_-|\ell m\rangle = C_-|\ell, m-1\rangle \qquad \ldots (3\text{–}51b)$$

Where C_+ and C_- are real numbers to be evaluated as in follow. By taking the conjugate of equation (3-51a) and multiplying the result by equation (3-51a) itself one obtain;

$$\langle\ell m|\hat{\ell}_-\hat{\ell}_+|\ell m\rangle = |C_+(\ell,m)|^2\langle\ell, m+1|\ell, m+1\rangle$$

$$= |C_+(\ell,m)|^2\delta_{\ell\ell}\delta_{m+1,m+1} = \langle\ell m|\hat{L}^2 - \hat{\ell}_z{}^2 - \hbar\hat{\ell}_z|\ell m\rangle$$

$$= |C_+(\ell,m)|^2 = \hbar^2\{\ell(\ell+1) - m^2 - m\}\,\delta_{\ell\ell}\delta_{mm}$$

$$\Rightarrow C_+(\ell,m) = \hbar\{(\ell-m)(\ell+m+1)\}^{1/2} \qquad \ldots (3\text{–}52a)$$

Similarly one can get;

$$C_-(\ell,m) = \hbar\{(\ell+m)(\ell-m+1)\}^{1/2} \qquad \ldots (3\text{–}52b)$$

Now one be able to precisely express x and y components of angular momentum. However, because;

$$\hat{\ell}_x = \frac{1}{2}(\hat{\ell}_+ + \hat{\ell}_-)$$

Thus;

$$\hat{\ell}_x|\ell m\rangle = \frac{1}{2}\{\hat{\ell}_+|\ell m\rangle + \hat{\ell}_-|\ell m\rangle\}$$

$$\hat{\ell}_x|\ell m\rangle = \frac{1}{2}\{C_+|\ell, m+1\rangle + C_-|\ell, m-1\rangle\} \qquad \ldots (3\text{–}53a)$$

In similar way one get;

$$\hat{\ell}_y|\ell m\rangle = \frac{-i}{2}\{C_+|\ell, m+1\rangle + C_-|\ell, m-1\rangle\} \qquad \ldots (3\text{–}53b)$$

Therefore, one may conclude that when $\hat{\ell}_x$ and $\hat{\ell}_y$ act upon state $|\ell m\rangle$ the result will either be the higher state $|\ell, m+1\rangle$ or the lower one $|\ell, m-1\rangle$ both with equal probability.

Remarks:

1) Since $\hat{L}^2$ is a hermitian operator, it is reliable, according to equation (3-42a), to say that; $\ell(\ell+1) \geq 0$. The reason behind is that as long as the form $\ell(\ell+1) = 0$ is concerned, one may found that either $\ell = 0$ or $\ell = -1$. But, apart from $\ell = 0$, the case $\ell = -1$ can never deduce $\ell(\ell+1) > 0$, so it must be rejected. Concerning with the case $\ell(\ell+1) > 0$, one obviously see the value $\ell = -1$ does not satisfy this inquiry although the remaining negative value does. But a singularity in the values of ℓ can never be accepted. So it is desirable to disregard all the negative values for ℓ and keep the positive ones in addition to the zero. Therefore one conclude that $\ell \geq 0$.
2) According to the overlap integral aspect one find that;

$$\langle \hat{\ell}_+(\ell m)|\hat{\ell}_+(\ell m)\rangle = \langle \ell m|\hat{\ell}_-\hat{\ell}_+|\ell m\rangle$$
$$= \langle \ell m|\hat{L}^2 - \hat{\ell}_z{}^2 - \hbar\hat{\ell}_z|\ell m\rangle$$
$$= \hbar^2\langle \ell m|\ell(\ell+1) - m^2 - m|\ell m\rangle$$
$$= \hbar^2\langle \ell m|\ell(\ell+1) - m(m+1)|\ell m\rangle$$
$$= \hbar^2\{\ell(\ell+1) - m(m+1)\} \geq 0 \qquad \text{. . . (3–54a)}$$

Similarly;

$$\langle \hat{\ell}_-(\ell m)|\hat{\ell}_-(\ell m)\rangle = \hbar^2\{\ell(\ell+1) - m(m-1)\} \geq 0 \qquad \text{. . . (3–54b)}$$

Thus;

$$\ell(\ell+1) \geq m(m+1) \qquad \text{. . . (3–55a)}$$
$$\ell(\ell+1) \geq m(m-1) \qquad \text{. . . (3–55b)}$$

Remember that $\ell \geq 0$, one logically deduce that;

$$-\ell \leq m \leq \ell$$

Thus values of m can only arranged between the limits $-\ell$ and ℓ.

3) Another approach could be adopted to verify that the higher and lower values of m are ℓ and $-\ell$, is as in follow. In accordance with equations (3-51) one get;

$$\hat{\ell}_+|\ell, m_{max}\rangle = 0 \;\text{ and }\; \hat{\ell}_-|\ell, m_{min}\rangle = 0$$

It follows respectively;

$$(\ell - m_{max})(\ell + m_{max} + 1) = 0$$

And

$$(\ell + m_{min})(\ell - m_{min} + 1) = 0$$

The solutions $m_{max} = -(\ell+1)$ and $m_{min} = (\ell+1)$ should be rejected since they doesn't achieve equations (3-55 b and a) respectively. While the solutions $m_{max} = \ell$ and $m_{min} = -\ell$ must accepted. Since the transition from m_{max} to m_{min}, and vice versa, can be done through a unit step that repeated by applying $\hat{\ell}_-$ and $\hat{\ell}_+$ respectively. There will be $2\ell + 1$ state as one graduate from $-\ell$ to $+\ell$ passing though the zero value. This means, however, a state ℓ being degenerated with degree $2\ell + 1$.

3-5-3 Matrices of Angular Momentum Operators

It should be mention that in some cases the representation of operators by matrices becomes a necessary mission. So, let us try to treat the angular momentum operator and start from the following commutation relation, see equations (3-41);

$$[\hat{L}^2, \hat{\ell}_z] = 0$$

This equation indicate that;

$$\langle \ell' m' | [\hat{L}^2, \hat{\ell}_z] | \ell m \rangle = 0$$

So;

$$\langle \hat{L}^2 \ell' m' | \hat{\ell}_z | \ell m \rangle - \langle \ell' m' | \hat{\ell}_z \hat{L}^2 | \ell m \rangle = 0$$

$$\hbar^2 \{\ell'(\ell'+1) - \ell(\ell+1)\} \langle \ell' m' | \hat{\ell}_z | \ell m \rangle = 0$$

It is seen that unless $\ell' = \ell$ the matrix element $\langle \ell' m' | \hat{\ell}_z | \ell m \rangle$ vanishes and hence $\hat{\ell}_z$ only have matrix elements between states that have the same angular momentum quantum numbers ℓ's. In other word states of different ℓ's are independent from each other. Strictly speaking, for state of specific ℓ' the corresponding angular momentum vector $\vec{L}$ will projected on ℓ_z by $2\ell' + 1$ different orientation depend on ℓ' and not any other one like ℓ. Indeed this conclusion is valid well for any operator that commute with $\hat{L}^2$. Anyway, regarding states of fixed ℓ, with the aid of equation (3-42b) the following equation may setup;

$$\langle \ell m' | \hat{\ell}_z | \ell m \rangle = m\hbar \delta_{m'm} \qquad \ldots (3\text{–}56)$$

Thus the matrix elements of $\hat{\ell}_z$ that differ from zero are those for which $m' = m$. However for $\ell = 1$ the $\hat{\ell}_z$ in matrix representation is;

$$\hat{\ell}_z = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \qquad \ldots (3\text{–}57)$$

Furthermore, with aid of equations (3-51) one may setup the following two equations;

$$\langle \ell m' | \hat{\ell}_+ | \ell m \rangle = C_+(\ell, m) \delta_{m', m+1} \qquad \ldots (3\text{–}58a)$$

$$\langle \ell m' | \hat{\ell}_- | \ell m \rangle = C_-(\ell, m)\delta_{m',m-1} \qquad \ldots \text{ (3–58b)}$$

It is seen that the non-zero matrix elements of $\hat{\ell}_+$ and $\hat{\ell}_-$ are those for which $m' = m + 1$ and $m' = m - 1$ respectivly. Keep in mind the values of $C_+(\ell, m)$ and $C_-(\ell, m)$ are as expressed in equations (3-52). So $\hat{\ell}_+$ and $\hat{\ell}_-$ in matrix notation are respectively as follows;

$$\hat{\ell}_+ = \hbar \begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix} \qquad \ldots \text{ (3–59a)}$$

$$\hat{\ell}_- = \hbar \begin{pmatrix} 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{pmatrix} \qquad \ldots \text{ (3–59b)}$$

So one has a method by means the matrix of any operator could be constructed.

H.W:

1) By using equations (3-53) find the matrix for of each of $\hat{\ell}_x$ and $\hat{\ell}_y$.

2) With aid of matrix form of $\hat{\ell}_+$ and $\hat{\ell}_-$ show that;

$$\hat{\ell}_x = \frac{1}{2}(\hat{\ell}_+ + \hat{\ell}_-) = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

And;

$$\hat{\ell}_y = \frac{1}{2}(\hat{\ell}_+ - \hat{\ell}_-) = \frac{i\hbar}{\sqrt{2}} \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}$$

3) Making use the matrix notion, verify the validity of relations (3-39).

3-6 Matrices Representation of Wave Functions

Let's consider, for example, the relation that define an operator $\hat{A}$. i.e.

$$|\psi\rangle = \hat{A}|\varphi\rangle \qquad \ldots \text{ (3–60)}$$

When the scalar product of this relation with any member of a complete set $|n\rangle$, say $|i\rangle$, is regarded one have;

$$\langle i|\psi\rangle = \langle i|\hat{A}|\varphi\rangle \qquad \ldots (3\text{–}61)$$

Insertion of unit operator appears in equation (3-11) between $\hat{A}$ and $|\varphi\rangle$ leads to the form;

$$\langle i|\psi\rangle = \sum_n \langle i|\hat{A}|\mathrm{n}\rangle\langle n|\varphi\rangle \qquad \ldots (3\text{–}62)$$

By writing $\langle i|\psi\rangle$ as a column matrix (vector) β_i and so $\langle n|\varphi\rangle$ as α_n one may set up the following two equations;

$$\langle i|\psi\rangle = \begin{pmatrix} \langle 1|\psi\rangle \\ \langle 2|\psi\rangle \\ \langle 3|\psi\rangle \\ \vdots \\ \langle i|\psi\rangle \end{pmatrix} \equiv \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \\ \vdots \\ \beta_i \end{pmatrix} \qquad \ldots (3\text{–}63)$$

And

$$\langle n|\varphi\rangle = \begin{pmatrix} \langle 1|\varphi\rangle \\ \langle 2|\varphi\rangle \\ \langle 3|\varphi\rangle \\ \vdots \\ \langle n|\varphi\rangle \end{pmatrix} \equiv \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \vdots \\ \alpha_n \end{pmatrix} \qquad \ldots (3\text{–}64)$$

Consequently, equation (3-62) becomes;

$$\beta_i = \sum_n \hat{A}_{in}\,\alpha_n \qquad \ldots (3\text{–}65a)$$

Or equivalently,

$$\begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \\ \vdots \\ \vdots \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & A_{13} \ldots \\ A_{21} & A_{22} & A_{23} \ldots \\ A_{31} & A_{32} & A_{33} \ldots \\ \ldots & \ldots & \ldots \quad \ldots \\ \ldots & \ldots & \ldots \ldots \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \vdots \\ \vdots \end{pmatrix} \qquad \ldots (3\text{–}65b)$$

The infinite dimensionality of these matrix equations is a consequence of the infinite dimensionality of Hilbert space. So, it should not make a confusion when a comparison with last three equations is carried out (***Explain***). However, finite matrix equations are relevant to vector spaces of finite dimension. Indeed, last equation proves that matrices could be used to represents both operators and kets (bras). However, since;

$$\langle n|\varphi\rangle^* = \langle\varphi|\mathrm{n}\rangle$$

It is convenient to write this equation as a row vector in the form;

$$\langle \varphi | n \rangle = (\alpha_1^* \quad \alpha_2^* \quad \alpha_3^* \cdots) \qquad \ldots (3\text{–}66)$$

Accordingly the scalar product $\langle \varphi | \psi \rangle$ can be written as;

$$\langle \varphi | \psi \rangle = \sum_n \langle \varphi | n \rangle \langle n | \psi \rangle$$

$$\langle \varphi | \psi \rangle = \sum_n \alpha_n^* \beta_n$$

$$\langle \varphi | \psi \rangle = (\alpha_1^* \quad \alpha_2^* \quad \alpha_3^* \cdots) \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \\ \vdots \end{pmatrix} \qquad \ldots (3\text{–}67)$$

3-7 Transformation Between Different Representations

In section (3-4) we talk about the possibility to represent an operator, like $\hat{A}$, in terms of two independent sets of biases namely $|v_n\rangle$ and $|u_n\rangle$. The first of them is considered to be an eigenkets for $\hat{A}$ while the other is not. Actually one may revise this situation for another operator like $\hat{B}$ The relation between these two representation has been established through the unitary transformation matrix, $U_{kn} = \langle u_k | v_n \rangle$. It seen that how could transform a representation of $\hat{A}$ in terms of $|v_n\rangle$ to its correspondence in terms of $|u_n\rangle$. So one may easily follow a same procedure to transform a representation of $\hat{B}$ in terms of $|v_n\rangle$.

Any state vector like $|\varphi\rangle$ can be expanded, and so operator like $\hat{A}$ could represented, in terms of these two different sets of biases. However, this section investigate the transformation between these two representations of both state vectors and operators.

3-7-1 Transformation of State Vectors

The expression of $|\varphi\rangle$ in terms of the set of biases $|v_n\rangle$ is given as;

$$|\varphi\rangle = \sum_m |v_m\rangle \langle v_m | \varphi \rangle$$

$$|\varphi\rangle = \sum_m \alpha_m |v_m\rangle \qquad \ldots (3\text{–}68a)$$

In matrix form;

$$|\varphi\rangle = \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \vdots \end{pmatrix} \qquad \ldots (3\text{–}68b)$$

In the representation of $|u_n\rangle$ the same state vector ($|\varphi\rangle$) is depicted as;

$$|\varphi\rangle = \sum_j |u_j\rangle\langle u_j|\varphi\rangle$$

$$|\varphi\rangle = \sum_j \beta_j |u_j\rangle \qquad \ldots (3\text{–}69a)$$

Which in matrix form reads as;

$$|\varphi\rangle = \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \\ \vdots \end{pmatrix} \qquad \ldots (3\text{–}69b)$$

Now, starting from the representation in terms of $|v_m\rangle$, we want to know the expression of the state vector $|\varphi\rangle$ in terms of the second representation ($|u_j\rangle$). Due to that an eigenket $|v_m\rangle$ can be expanded in terms of the biases $|u_j\rangle$ and hence equation (3-68a) becomes;

$$|\varphi\rangle = \sum_{m,j} \alpha_m |u_j\rangle\langle u_j|v_m\rangle$$

$$|\varphi\rangle = \sum_{m,j} \alpha_m U_{jm} |u_j\rangle \qquad \ldots (3\text{–}70)$$

Where $U_{jm} = \langle u_j|v_m\rangle$ is the unitary transformation matrix. The comparison between equations (3-70) and (3-69a) reveals that;

$$\beta_j = \sum_m \alpha_m U_{jm} \qquad \ldots (3\text{–}71a)$$

H.W: Verify the validity of equation ((3-71a).

Anyway equation (3-71a) gives the relation between two different representations for the same state vector. In matrix form this equation can be written as;

$$\begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \\ \vdots \\ \beta_j \end{pmatrix} = \begin{pmatrix} U_{11} & U_{12} & U_{13} \ldots \\ U_{21} & U_{22} & U_{23} \ldots \\ U_{31} & U_{32} & U_{33} \ldots \\ \ldots & \ldots & \ldots \quad \ldots \\ U_{j1} & U_{j2} & U_{j3} \ldots \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \vdots \\ \alpha_m \end{pmatrix} \qquad \ldots (3\text{–}71b)$$

Or equivalently;

$$\varphi^u = U\varphi^v$$

H.W: Show that by starting from the representation in terms of $|u_i\rangle$ for the state vector $|\varphi\rangle$ one can deduce its representation in terms of $|v_n\rangle$ to be as;

$$\alpha_n = \sum_i \beta_i U^{\dagger}_{ni} \qquad \ldots (3\text{–}72a)$$

In matrix form equation (3-72a) written as;

$$\begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \vdots \\ \alpha_n \end{pmatrix} = \begin{pmatrix} U^{\dagger}_{11} & U^{\dagger}_{12} & U^{\dagger}_{13} \cdots \\ U^{\dagger}_{21} & U^{\dagger}_{22} & U^{\dagger}_{23} \cdots \\ U^{\dagger}_{31} & U^{\dagger}_{32} & U^{\dagger}_{33} \cdots \\ \cdots & \cdots & \cdots \quad \cdots \\ U^{\dagger}_{n1} & U^{\dagger}_{n2} & U^{\dagger}_{n3} \cdots \end{pmatrix} \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \\ \vdots \\ \beta_i \end{pmatrix} \qquad \ldots (3\text{–}72b)$$

Or equivalently; $\varphi^v = U^{\dagger}\varphi^u$.

3-7-2 Transformation of Operators

According to equation (3-68) the matrix elements of an operator $\hat{A}$, by means of an arbitrary two state vectors ($|\varphi\rangle$and $|\psi\rangle$), can be written as follows;

$$\langle\varphi|\hat{A}|\psi\rangle = \sum_{n,m}\langle\varphi|n\rangle\langle n|\hat{A}|m\rangle\,\langle m|\psi\rangle$$

$$\langle\varphi|\hat{A}|\psi\rangle = \sum_{n,m} \alpha_n^*\, A_{nm}\tilde{\alpha}_m \qquad \ldots (3\text{–}73a)$$

Which means that;

$$\langle\varphi|\hat{A}|\psi\rangle = (\alpha_1^* \quad \alpha_2^* \quad \ldots \alpha_n^*) \begin{pmatrix} A_{11} & A_{12} & A_{13} \cdots \\ A_{21} & A_{22} & A_{23} \cdots \\ A_{31} & A_{32} & A_{33} \cdots \\ \cdots & \cdots & \cdots \quad \cdots \\ A_{n1} & A_{n2} & A_{n3} \cdots \end{pmatrix} \begin{pmatrix} \tilde{\alpha}_1 \\ \tilde{\alpha}_2 \\ \tilde{\alpha}_3 \\ \vdots \\ \tilde{\alpha}_m \end{pmatrix} \qquad \ldots (3\text{–}73b)$$

It is well known that expectation value is a special case for the last equation, so it may written as;

$$\langle\varphi|\hat{A}|\varphi\rangle = \sum_{n,m}\langle\varphi|n\rangle\langle n|\hat{A}|m\rangle\,\langle m|\varphi\rangle$$

$$\langle\varphi|\hat{A}|\varphi\rangle = \sum_{n,m} \alpha_n^* A_{nm}\alpha_m \qquad \text{. . . (3–74a)}$$

Or equivalently;

$$\langle\varphi|\hat{A}|\varphi\rangle = (\alpha_1^* \quad \alpha_2^* \quad \dots \alpha_n^*)\begin{pmatrix} A_{11} & A_{12} & A_{13} \dots \\ A_{21} & A_{22} & A_{23} \dots \\ A_{31} & A_{32} & A_{33} \dots \\ \dots & \dots & \dots \dots \\ A_{n1} & A_{n2} & A_{n3} \dots \end{pmatrix}\begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \vdots \\ \alpha_m \end{pmatrix}$$

. . . (3–74b)

Equation (3-73 and 74) gives an evidence for the fact that, the diagonal elements of any operator's matrix are corresponds to expectation values of that operator over all of the ket vectors (biases), by means a given state vector is expanded. Obviously both of operator $\hat{A}$ and state vector $|\varphi\rangle$ are represented in terms of the orthonormal set (biases) $|n\rangle$. Anyway, there are only two cases of the arbitrary state vector ($|\varphi\rangle$) can be taken into account that are, either it being expanded in terms of an eigenkets $|v_n\rangle$for operator $\hat{A}$ (recall equation (3-68)) or conversely in terms of not eigenkets $|u_i\rangle$ for this operator (recall equation (3-69)).

Case-I: V-Representation

Concerning with such a case the state vector $|\varphi\rangle$ being expanded in terms of the set $|v_n\rangle$, which is an eigenkets vectors for the operator $\hat{A}$. So equation (3-74a) becomes;

$$\langle\varphi|\hat{A}|\varphi\rangle = \sum_{n,m}\langle\varphi|v_n\rangle\langle v_n|\hat{A}|v_m\rangle\,\langle v_m|\varphi\rangle$$

$$\langle\varphi|\hat{A}|\varphi\rangle = \sum_{n,m} \alpha_n^* A_{nm}\alpha_m \qquad \text{. . . (3–75a)}$$

$$\langle\varphi|\hat{A}|\varphi\rangle = \sum_{n,m} \alpha_n^* a_m\delta_{nm}\alpha_n$$

$$\langle\varphi|\hat{A}|\varphi\rangle = \sum_n \alpha_n^* a_n\alpha_n$$

In matrix form;

$$\langle\varphi|\hat{A}|\varphi\rangle = (\alpha_1^* \quad \alpha_2^* \quad \dots \alpha_n^*) \begin{pmatrix} a_1 & 0 & 0 \dots \dots \dots \\ 0 & a_2 & 0 \dots \dots \dots \\ 0 & 0 & a_3 \;\; \dots \dots \\ \dots & \dots & \dots \;\; \dots \;\; \dots \\ 0 & 0 & 0 \;\; \dots \;\; a_n \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \vdots \\ \alpha_n \end{pmatrix}$$

. . . (3–75b)

It is worth to mention that for such a case the projection of state vector $|\varphi\rangle$ on any eigenket vector $|v_k\rangle$ has a probability $|\langle v_k|\varphi\rangle|^2$, since an expectation value govern all of the allowed states of a quantum mechanical system. Actually equation (3-75) state that a measurement for the observable A has been carried out, and hence the probable results a_n are distributed among all of the admissible states (kets) of the system (space) with a probability $|\alpha_n|^2$. Since the probability is conserved in a system of a stationary states it follows that $\sum_n |\alpha_n|^2 = 1$.

H.W:

i- Derive with explanation why the scalar product ends to the unit value for each of the admissible state. i.e. $\sum_n \alpha_n^* \, \alpha_n = 1$.

ii- set the expression in (**i**) in matrix form.

Case-II: U-Representation

The state vector $|\varphi\rangle$ will expanded now in terms of the orthonormal set (biases) $|u_i\rangle$ which is not an eigenkets for the operator $\hat{A}$. So equation (3-74a) can be written as;

$$\langle\varphi|\hat{A}|\varphi\rangle = \sum_{i,j} \langle\varphi|u_i\rangle\langle u_i|\hat{A}|u_j\rangle \, \langle u_j|\varphi\rangle$$

$$\langle\varphi|\hat{A}|\varphi\rangle = \sum_{i.j} \beta_i^* \, A_{ij}\beta_j$$

$$\langle\varphi|\hat{A}|\varphi\rangle = \sum_{i.j} \beta_i^* \, \tilde{A}_{ij}\beta_j \qquad \dots \text{(3–76a)}$$

In matrix form;

$$\langle\varphi|\hat{A}|\psi\rangle = (\beta_1^* \quad \beta_2^* \quad \dots\beta_i^*)\begin{pmatrix}\tilde{A}_{11} & \tilde{A}_{12} & \tilde{A}_{13}\dots \\ \tilde{A}_{21} & \tilde{A}_{22} & \tilde{A}_{23}\dots \\ \tilde{A}_{31} & \tilde{A}_{32} & \tilde{A}_{33}\dots \\ \dots & \dots & \dots \quad \dots \\ \tilde{A}_{i1} & \tilde{A}_{i2} & \tilde{A}_{i3}\dots\end{pmatrix}\begin{pmatrix}\beta_1 \\ \beta_2 \\ \beta_3 \\ \vdots \\ \beta_j\end{pmatrix}$$

. . . (3–76b)

The matrix elements in this representation are nominated by $\tilde{A}_{ij}$ in order to make a clear distinguish over its counterpart in V-representation **(Why?)**.

Let's now make a transformation from U-representation to V-representation starting from equation (3-76a). This equation with aid of equation (3-71a) can be re-written in the form;

$$\langle\varphi|\hat{A}|\varphi\rangle = \sum_{i.j}\{\sum_{n,m}\alpha_n^* U_{in}^* \tilde{A}_{ij}\alpha_m U_{jm}\}$$

$$\langle\varphi|\hat{A}|\varphi\rangle = \sum_{i.j}\{\sum_{n,m}\alpha_n^* U_{ni}^\dagger \tilde{A}_{ij}U_{jm}\alpha_m\}$$

$$\langle\varphi|\hat{A}|\varphi\rangle = \sum_{n,m}\alpha_n^*\{\sum_{i,j} U_{ni}^\dagger \tilde{A}_{ij}U_{jm}\}\alpha_m$$

$$\langle\varphi|\hat{A}|\varphi\rangle = \sum_{n,m}\alpha_n^*\left(U^\dagger\tilde{A}U\right)_{nm}\alpha_m \qquad \dots (3\text{–}77)$$

The result of comparison between equations (3-77 and 75a) leads to the following formula;

$$a_m\delta_{nm} = A_{nm} = \left(U^\dagger\tilde{A}U\right)_{nm} \qquad \dots (3\text{–}77a)$$

Or;

$$a_m\delta_{nm} = A_{nm} = \sum_{i,j} U_{ni}^\dagger \tilde{A}_{ij}U_{jm} \qquad \dots (3\text{–}77b)$$

Generally one may write;

$$\hat{A} = U^\dagger\hat{\tilde{A}}U$$

Equation (3-77) is exactly similar to equation (3-33) and so a transformation for the matrix elements of the operator $\hat{A}$ has been carried out from the space $|v_n\rangle$ to the space $|u_n\rangle$. In other word a diagonalizaition process for the operator $\hat{A}$ is implemented by means of the unitary transformation matrix U_{in}.

Starting from equation (3-75a) with aid of equation (3-72a) one may use a similar approach to make a transformation from U-representation to the V-representation as follows;

$$\langle\varphi|\hat{A}|\varphi\rangle = \sum_{n,m} \alpha_n^* A_{nm}\alpha_m$$

$$\langle\varphi|\hat{A}|\varphi\rangle = \sum_{n,m}\{\sum_{i,j} \beta_i^* (U_{ni}^\dagger)^* A_{nm}\beta_j U_{mj}^\dagger\}$$

$$\langle\varphi|\hat{A}|\varphi\rangle = \sum_{n,m}\{\sum_{i,j} \beta_i^* U_{in} A_{nm} U_{mj}^\dagger \beta_j\}$$

$$\langle\varphi|\hat{A}|\varphi\rangle = \sum_{i,j} \beta_i^* \{\sum_{n,m} U_{in} A_{nm} U_{mj}^\dagger\}\beta_j$$

$$\langle\varphi|\hat{A}|\varphi\rangle = \sum_{i,j} \beta_i^* (UAU^\dagger)_{i,j}\beta_j \qquad \ldots (3\text{–}78)$$

The comparison between equations (3-78 and 76a) reveals that;

$$\tilde{A}_{ij} = (UAU^\dagger)_{ij} \qquad \ldots (3\text{–}79a)$$

Or;

$$\tilde{A}_{ij} = \sum_{n,m} U_{in} A_{nm} U_{mj}^\dagger \qquad \ldots (3\text{–}79b)$$

In general;

$$\hat{\tilde{A}} = U\hat{A}U^\dagger$$

H.W:

i- Starting from equation (3-76a) deduce the expression in equation (3-75a).

ii- Prove that; $[U, U^\dagger] = 0$.

iii- Verify at which condition the matrix of operator $\tilde{A}_{ij}$ become diagonal.

iv- Show that the probability distribution identity, $\sum_n \alpha_n^* \alpha_n = 1$, can be written implicitly as; $\sum_i \alpha_i^{(n)*} \alpha_i^{(m)} = \delta_{nm}$, where the set $\alpha_i^{(n)}$ is assumed to belong to the eigen value a_n.

v-Show that the probability distribution formula in (**iv**) may implies the aspect of degeneracy.

vi- Show that the probability distribution formula in (**iv**) involve that the eigen vectors for each eigen value being normalized.

3-8 Eigen Values (Vectors) Determination

Obviously an eigen value equation is a special case for equation (3-60) which in turn can be written as;

$$\hat{A}|\varphi\rangle = a|\varphi\rangle \qquad \ldots (3\text{–}80)$$

Indeed this equation describe a definite measurement process for the observable A in state vector $|\varphi\rangle$, however, the result is an eigen value a. Equation (3-80) implies that either the state vector $|\varphi\rangle$ is one of the complete eigenket vectors $|n\rangle$, so a must tend to be any of a_n, or the eigen value a belong to the projection of $\hat{A}$ over all of the eigenkets vectors $|n\rangle$. The latter case involves the degeneracy for the state vector $|\varphi\rangle$ that has an eigen value a. Let's ignore the degeneracy and focus attention for the former case. Accordingly equation (3-80) can be written as;

H.W:

$$\sum_j A_{ij}\,\alpha_j = a\alpha_i, \;\; deg. \qquad \ldots (3\text{–}81)$$

$$\sum_j A_{ij}\,\alpha_j^{(n)} = a_n\alpha_i^{(n)}, non\; deg. \qquad \ldots (3\text{–}82a)$$

In matrix form equation (3-82) can be written as;

$$\begin{pmatrix} A_{11} & A_{12} & \ldots A_{1j} \\ A_{21} & A_{22} & \ldots A_{2j} \\ \cdots\cdots & \cdots\cdots & \cdots\cdots \\ A_{i1} & A_{i2} & \ldots A_{ij} \end{pmatrix} \begin{pmatrix} \alpha_1^n \\ \alpha_2^n \\ \vdots \\ \alpha_j^n \end{pmatrix} = a_n \begin{pmatrix} \alpha_1^n \\ \alpha_2^n \\ \vdots \\ \alpha_i^n \end{pmatrix} \qquad \ldots (3\text{–}82b)$$

Equation (3-82a) can be written as;

$$\sum_j (A_{ij} - a_n\delta_{ij})\alpha_j^{(n)} = 0 \qquad \ldots (3\text{–}83a)$$

In matrix form equation (3-83) becomes as;

$$\begin{pmatrix} A_{11} - a_n & A_{12} & \ldots A_{1j} \\ A_{21} & A_{22} - a_n & \ldots A_{2j} \\ \cdots\cdots & \cdots\cdots & \cdots\cdots \\ A_{i1} & A_{i2} & \ldots A_{ij} - a_n \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_i \end{pmatrix} = 0 \qquad \ldots (3\text{–}83b)$$

Keep in mind $\alpha_i^{(n)} \equiv \alpha_i$ belong to the eigen value a_n. According to theory of matrices there will be a non-trivial solution for this system of equations,

$(i \times j)$ matrix, if and only if when the determinant of this matrix being null. i.e.

$$det|A_{ij} - a_n \delta_{ij}| = 0 \qquad \ldots (3\text{–}84)$$

The solution of equation (3-84) gives an algebraic equation of a_n of i-power when the matrix of $\hat{A}$ become square matrix. By solving this set of equations one can find the eigen values of $\hat{A}$ to be the roots of the algebraic equation $a_n^1, a_n^2, a_n^3, \ldots, a_n^i$. Just the eigen values being well defined the correspondence eigen vectors can be found from equation (3-83a).

Actually this is an efficient approach for finding eigen values and their correspondent eigen vectors for operators that represented by finite matrices. However, this is not so simple for infinite matrices which equivalent to solving Schrodinger equation.

Indeed what we have been did so for is that the following system of equations is setup;

$$\begin{pmatrix} a_1 & 0 & \ldots 0 \\ 0 & a_2 & \ldots 0 \\ \ldots\ldots & \ldots\ldots & \ldots\ldots \\ 0 & 0 & \ldots a_n \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{pmatrix} = \lambda \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{pmatrix} \qquad \ldots (3\text{–}85)$$

Thus one obviously seen that λ are $a_1, a_2, a_3, \ldots, a_n$ and the corresponding orthonormalized eigenvectors are;

$$u_1 = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, u_2 = \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix}, \ldots, u_n = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix}$$

Example: Determine the eigen values and the normalized eigenvectors for the operator matrix shown below and then find the unitary matrix that diagonalizes it.

$$\hat{A} = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Solution:

According to the relation; $\sum_i A_{ij}\,\alpha_j = \lambda\alpha_i$ we have;

$$\begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{pmatrix} = \lambda\begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{pmatrix}$$

The eigen values of $\hat{A}$ can be determined either by letting;

$$\begin{vmatrix} 0-\lambda & -i & 0 \\ i & 0-\lambda & 0 \\ 0 & 0 & 0-\lambda \end{vmatrix} = 0$$

Or by setup the following relations;

$$-i\alpha_2 = \lambda\alpha_1 \qquad \text{....(3-86a)}$$

$$i\alpha_1 = \lambda\alpha_2 \qquad \text{....(3-86b)}$$

$$0 = \lambda\alpha_3 \qquad \text{....(3-86c)}$$

Both of these two ways approaches leads to that λ being either (0) or (1) or (-1). So the eigen vectors corresponds to each of these eigen values may deduced as follows;

i) When $\lambda = 0 \xrightarrow{yields} \alpha_1 = \alpha_2 = 0$ and hence $\alpha_3 = 1$ due to $|\alpha_1|^2 + |\alpha_2|^2 + |\alpha_3|^2 = 1$. i.e. $(0 \quad 0 \quad 1)$.

ii)When $\lambda = 1 \xrightarrow{yields} \alpha_1 = \frac{1}{\sqrt{2}}, \alpha_2 = \frac{i}{\sqrt{2}}$ *and* $\alpha_3 = 0$ due to the same reason. i.e. $\left(\frac{1}{\sqrt{2}} \quad \frac{i}{\sqrt{2}} \quad 0\right)$.

iii) When $\lambda = -1 \xrightarrow{yields} \alpha_1 = \frac{1}{\sqrt{2}}, \alpha_2 = \frac{-i}{\sqrt{2}}$ *and* $\alpha_3 = 0$ due to the normalization condition. i.e. $\left(\frac{1}{\sqrt{2}} \quad \frac{-i}{\sqrt{2}} \quad 0\right)$.

Therefore, the following eigen vectors; $\begin{pmatrix}0\\0\\1\end{pmatrix}$, $\begin{pmatrix}\frac{1}{\sqrt{2}}\\\frac{i}{\sqrt{2}}\\0\end{pmatrix}$ and $\begin{pmatrix}\frac{1}{\sqrt{2}}\\\frac{-i}{\sqrt{2}}\\0\end{pmatrix}$ are respectively correspondence to the eigen values $\lambda = 0,1,-1$. So the matrix that diagonalize $\hat{A}$ is;

$$U = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 0 & 1\\ i & 0 & -i\\ 0 & \sqrt{2} & 0\end{pmatrix}$$

H.W:

1) for the above example find $U^\dagger$ and then verify the relation; $U^\dagger U = 1$. **2)** Show that the deduced eigen vectors are orthonormalized.

3-9 Density Operator

So far considerations have been carried out to deals with analysis of a single state, i.e. pure state or single system. Such a state can be expanded in terms of a complete orthonormal basis (Eigen kets$|u_n\rangle$) as shown in equation (3-1). i.e.

$$|\varphi\rangle = \sum_n c_n\,|u_n\rangle \qquad \ldots\ (3\text{–}1)$$

Indeed any measurement may implement upon this state aims at find out what the possible measurement results are on the system, and hence define the probability of obtaining each of possible result.

According to statistical point of view it often desirable to investigate a collection (large number) of systems (ensemble or mixed states) rather than considering a single pure quantum system. In other word, several or either many members of an ensemble may be found in more than two different quantum states, with a certain probability that a member of the ensemble is found in each of these states. Strictly speaking the members of the ensemble are the states$|\varphi_1\rangle$, $|\varphi_2\rangle$, $|\varphi_3\rangle$, …, $|\varphi_n\rangle$ and so the probability of finding each state is respectively represented by $p_1, p_2, \ldots, p_n$. This sort of quantum mechanical situation (mixture of states) is describe by means of a density operator rather than a wave function.

However, density operator is an alternate representation of the state of a quantum composite system for which we have previously used the wave function. i.e. density operator is equivalent to using the wave and it is usually represented by the symbol ρ.

Consequently the density operator that represents a collection of states $|\varphi_1\rangle, |\varphi_2\rangle, |\varphi_3\rangle, \ldots |\varphi_n\rangle$ expressed by the following formula;

$$\rho = \sum_n p_n |\varphi_n\rangle\langle\varphi_n| \qquad \ldots (3\text{–}87)$$

However, for the case when the state of an ensemble is known exactly (pure state), this means that the state is a single, say $|\varphi_i\rangle\rangle$. Hence p_i=1 and all others probabilities are vanishes, i.e. $p_{n\neq i}$=0. Consequently, equation (3-87) becomes;

$$\rho = |\varphi_i\rangle\langle\varphi_i| \qquad \ldots (3\text{–}88a)$$

Qr equivalently;

$$\rho = |\varphi\rangle\langle\varphi| \qquad \ldots (3\text{–}88b)$$

Which is a projector operator that own all of the properties argued previously in section (3-2). So, for a pure state density operator may be defined as an outer product of the pure state with its own conjugate.

H.W:

1- Prove that the density operator appear in equation (3-88b) satisfies the properties of projection operator.

2- Concerning with the physical meaning compare between equations (3-87 and 88).

3-10 Density Operator for a Pure State

Apparently the density operator is an average operator that allows the description of a statistical mixture of an ensemble. For the case of a pure state its function reduces to an outer product for the state. Let's now tries to find whether there is a relation being exist between density operator and the expectation value. It is obvious (see equation (3-14)) that the expectation value or average of an observable A with respect to a pure state $|\psi\rangle$ may be expressed as;

$$\langle A\rangle = \langle\psi|\hat{A}|\psi\rangle = \sum_{n,m} c_n^* \, c_m A_{nm} \qquad \ldots \ (3\text{–}89)$$

Recall equation (3-2) last formula can be written as follows;

$$\langle A\rangle = \langle\psi|\hat{A}|\psi\rangle = \sum_{n,m}\langle\psi|u_n\rangle\,\langle u_m|\psi\rangle A_{nm} \qquad \ldots \ (3\text{–}90)$$

Since $\langle u_n|\psi\rangle$ is just a complex number, last equation convert to;

$$\langle A\rangle = \langle\psi|\hat{A}|\psi\rangle = \sum_{n,m}\langle u_m|\psi\rangle\langle\psi|u_n\rangle\, A_{nm} \qquad \ldots \ (3\text{–}91)$$

According to equation (3-88b) one get;

$$\langle A\rangle = \langle\psi|\hat{A}|\psi\rangle = \sum_{n,m}\langle u_m|\rho|u_n\rangle A_{nm} \qquad \ldots \ (3\text{–}92)$$

Similarly;

$$\langle A\rangle = \langle\psi|\hat{A}|\psi\rangle = \sum_{n,m}\langle u_m|\rho|u_n\rangle\langle u_n|A|u_m\rangle \ldots \ (3\text{–}93)$$

Making use the closure relation one get;

$$\langle A\rangle = \langle\psi|\hat{A}|\psi\rangle = \sum_{m}\langle u_m|\rho A|u_m\rangle \qquad \ldots \ (3\text{–}94)$$

Recall equation (3-35) the following formula may set up;

$$\langle A\rangle = \langle\psi|\hat{A}|\psi\rangle = Tr(\rho A) \qquad \ldots \ (3\text{–}95)$$

An important conclusion can be read from the last equation that is; *the expectation value could successfully calculated by means of the density operator.*

H.W: Prove that; $Tr(\rho) = 1$ and then state the physical meaning of such formula.

3-11 Properties of Density Operator

1- The density operator is Hermitian, $\rho = \rho^\dagger$.
2- The trace of any density matrix is equal to one, $Tr(\rho) = 1$.
3- For a pure state, since $\rho^2 = \rho$, $Tr(\rho^2) = 1$.
4- Time evaluation of density operator is given by, $i\hbar \frac{d\rho}{dt} = [\hat{H}, \rho]$.
5- The expectation value of an operator A can be calculated using $\langle A \rangle = \langle \psi | \hat{A} | \psi \rangle = Tr(\rho A)$.

3-12 Selection Rules

Transition in certain dynamical variable from a specific state to another different one is not always possible. So, it is important to know the procedure by which these transitions are allowed or not. For example one may start with a molecule modulated to be a harmonic oscillator since it is a simple one. However, this may corresponds to absorption or transmission of infrared radiation. The question now is what the restrictions in the transition of the dipole moment for the case under consideration. Initially, lets neglect the rotational and consider vibration transitions and start with expanding μ by McLaren's series around the equilibrium nucleus separation as follows;

$$\mu(x) = \mu(x_0) + \mu'(x_0) \cdot x + \cdots \quad \Longrightarrow$$

What the physical meaning that could be realized from this expansion?

Then the dipole moment transition considering the first two terms is;

$$\mu_{nm} = \langle n | \hat{\mu} | m \rangle$$

$$\mu_{nm} = \langle n | \mu_0 | m \rangle + \mu_0' \langle n | \hat{x} | m \rangle$$

$$\mu_{nm} = \mu_0 \delta_{nm} + C \langle n | (\hat{a}^+ + \hat{a}) | m \rangle$$

$$\mu_{nm} = C\langle n|(\hat{a}^{+}+\hat{a})|m\rangle \qquad \text{where} \qquad C = \mu_0(\hbar/2m\omega)^{1/2}$$

$$\mu_{nm} = C\{\langle n|\hat{a}^{+}|m\rangle + \langle n|\hat{a}|m\rangle\}$$

$$\mu_{nm} = C\{\sqrt{m+1}\langle n|m+1\rangle + \sqrt{m}\langle n|m-1\rangle\}$$

$$\mu_{nm} = C\{\sqrt{m+1}\delta_{n,m+1} + \sqrt{m}\delta_{n,m-1}\}$$

So the only non-zero matrix element are those for which m=n±1. Hence the selection rules for these transitions are;

$$\boxed{\Delta n = \pm 1}$$

Concerning with the rotational transitions a similar approach can be followed if a diatomic molecule is modulated as a rigid rotator. Typically, this situation will govern the transitions and absorption in the range of far infrared or microwave radiation. For simplicity one may assume that the field is polarized in one dimension, say z, for example. Then dipole moment will take the form;

$$\mu = \mu_0 \cos\theta$$

Which direction is this?

So,

$$\mu_{l'm',lm} = \langle l'm'|\hat{\mu}|lm\rangle$$

$$\mu_{l'm',lm} = \mu_0\langle l'm'|\cos\theta|lm\rangle$$

Making use the identity;

$$\cos\theta\,|l,m\rangle = a_\ell^m\,|l-1,m\rangle + b_\ell^m\,|l+1,m\rangle$$

One can directly obtain;

$$\mu_{l'm',lm} = \mu_0\, a_\ell^m\langle l'm'|l-1,m\rangle + \mu_0\, b_\ell^m\langle l',m'|l+1,m\rangle$$

$$\mu_{l'm',lm} = \mu_0\, a_\ell^m\,\delta_{m'm}\delta_{l',l-1} + \mu_0\, b_\ell^m\,\delta_{m'm}\delta_{l',l+1}$$

It can be seen that the non-zero matrix element of μ are those for which;

$\boxed{\Delta m = 0}$ and $\boxed{\Delta l = \pm 1}$

Which are the selection rules for rigid rotator.

H.W:

Deduce the dipole moment selection rules for a molecule considering its rotation and vibration motion together. ***Hint; Use the assumption*** $\mu(x) = (a + b \cdot x)\cos\theta$ where a and b are constants.

Exercises:

1) The y-component of the angular momentum may given by the following expression; $\hat{\ell}_y = i\hbar\left(-cos\varphi \frac{\partial}{\partial\theta} + cot\theta\, sin\varphi \frac{\partial}{\partial\varphi}\right)$. By assume the following spherical harmonics; $|u_1\rangle = Y_1^1 = -\sqrt{\frac{3}{8\pi}} sin\theta e^{i\varphi}$, $|u_2\rangle = Y_1^0 = \sqrt{\frac{3}{4\pi}} cos\theta$ and $|u_3\rangle = Y_1^{-1} = \sqrt{\frac{3}{8\pi}} sin\theta e^{-i\varphi}$ as a ket vectors (biases) for the representation requirements find;

i- The matrix form of this operator.

ii- The eigen values and their corresponding eigen vectors for this operator.

2) Concerning with harmonic oscillator system determine $\langle H\rangle, \langle x^2\rangle$ and $\langle x\rangle$ for the state vector; $\psi = \frac{1}{\sqrt{6}}(1 \quad 2 \quad 1 \quad 0 \ldots)$.

3) For the Hermitian matrix;

$$A = \begin{pmatrix} -3 & \sqrt{\frac{19}{4}} e^{i\pi/3} \\ \sqrt{\frac{19}{4}} e^{-i\pi/3} & 6 \end{pmatrix}$$

i- Determine the eigen values and eigen vectors.

ii- Determine the matrix U that diagonalizes A.